

=> fil reg

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STRUCTURE FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7
 DICTIONARY FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

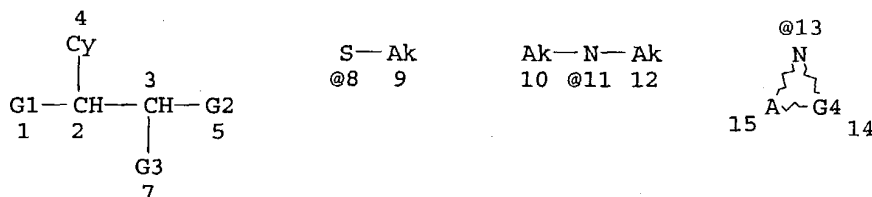
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 127

L12 STR



VAR G1=11/13

VAR G2=S/8

VAR G3=AK/CB

REP G4=(1-6) A

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

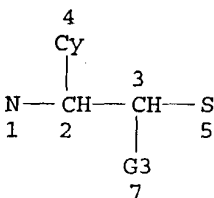
RSPEC 13

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L21 SCR 1164

L23 STR



VAR G3=AK/CB

NODE ATTRIBUTES:

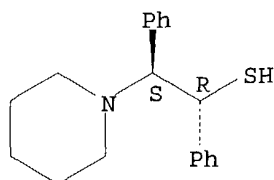
NSPEC IS RC AT 1

DEFAULT MLEVEL IS ATOM

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ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:39785 CAPLUS
DOCUMENT NUMBER: 126:131036
TITLE: Chiral β -amino thiol catalysts for the
enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong
Soo; Kim, Joo In
CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996),
17(12), 1135-1142
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of diethylzinc with α -branched aldehydes in the presence of
a catalytic amount (5 mol %) of various β -amino thiols in toluene or
ether provided the corresponding secondary alcs. in outstanding ee.
Detailed preparative procedure for the β -amino thiols are presented.
IT 160011-80-3P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc to aldehydes using chiral
 β -amino thiol catalysts)
RN 160011-80-3 CAPLUS
CN 1-Piperidineethanethiol, α,β -diphenyl-, ($\alpha R,\beta S$)-
(9CI) (CA INDEX NAME)

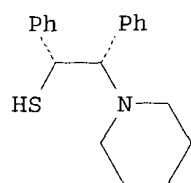
Absolute stereochemistry. Rotation (-).



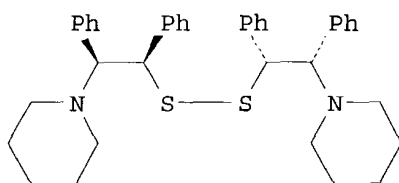
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:194984 CAPLUS
DOCUMENT NUMBER: 122:55341
TITLE: Enantioselective addition of diethylzinc to aldehydes
catalyzed by a drug-unrelated chiral amino thiol and
the corresponding disulfide
AUTHOR(S): Kang, Jahyo; Kim, Dong Soo; Kim, Joo In
CORPORATE SOURCE: Department Chemistry, Sogang University, Seoul,
121-742, S. Korea
SOURCE: Synlett (1994), (10), 842-4
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:55341
GI

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I



II

AB Reaction of diethylzinc with aldehydes in the presence of a catalytic amount of a β -amino thiol I (5 mol %) and the disulfide II (2.5 mol %) in toluene at 0° provided the corresponding secondary alcs. in excellent ee's.

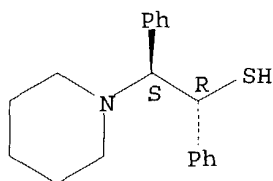
IT 160011-80-3P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc with aldehydes catalyzed by chiral amino thiol and disulfide)

RN 160011-80-3 CAPLUS

CN 1-Piperidineethanethiol, α,β -diphenyl-, ($\alpha R,\beta S$)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:531411 CAPLUS

DOCUMENT NUMBER: 113:131411

TITLE: Concerning mass spectra of β -heterosubstituted thioethers

AUTHOR(S): Carreno, M. Carmen; Carretero, Juan C.; Garcia Ruano, Jose L.; Martinez, M. Carmen

CORPORATE SOURCE: Dep. Quim., Univ. Auton. Madrid, Madrid, 28049, Spain

SOURCE: Organic Mass Spectrometry (1990), 25(6), 339-42

CODEN: ORMSBG; ISSN: 0030-493X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The mass spectra of 32 erythro- and threo-RCHXCHRSMe (R = Me, Ph; X = F, Cl, Br, iodo, OH, OMe, OAc, NH₂, NMe₂) were interpreted in detail. Linear free-energy relationships were determined between the ratio of the relative abundances of the RCHX⁺ and RCHSMe⁺ peaks and the inductive and resonance σ consts. of X.

IT 97241-47-9

RL: PRP (Properties)
(mass spectrum of)

RN 97241-47-9 CAPLUS

CN Benzeneethanamine, N,N-dimethyl- β -(methylthio)- α -phenyl-,
(R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

